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Predictive Science Academic Alliance Program (PSAAP)
Guidelines for Applications of Interest

A new competition to launch major research centers and collaborative research efforts is underway. The purpose is to advance the state-of-the-art by establishing validated, large-scale, multidisciplinary, simulation-based "Predictive Science" as a major academic and applied research focus area. Each center will be expected to have a flagship "grand challenge" multi-year simulation objective that will push the boundaries of current computational science and physical modeling capabilities in an area of programmatic interest to the National Nuclear Security Administration (NNSA) Laboratories.

Predictive Science is defined as the development and application of verified and validated (V&V) computational simulations to predict the properties and dynamic response of complex systems particularly in cases where routine, separable, experimental tests, while important, are difficult. This general idea can be extended to a wide variety of scientific and engineering applications, including biological systems, global economics, nuclear weapons effects, climate modeling, to efficient manufacturing including nuclear weapons, flexible and agile manufacturing, optimized materials by design, etc. In all these areas, computer simulations require robust mathematical models that integrate science-based models or algorithms from a diverse set of disciplines; each discipline standing, in its own right, as an important element of many applications. Success requires both software and algorithmic advances for integrating effective treatment of multiple physical processes into a single simulation that is truly predictive. The complexity of these applications and the associated simulations requires effective utilization of the most powerful computing systems available. Finally, since the final test of the scientific enterprise is prediction via validated simulations, predictions derived from such simulations must be strongly connected with experimental and/or observational data including the possibility of designing and conducting novel experiments or observations.

As defined, Predictive Science is a broadly-based predictive strategy. However, the PSAAP program will be focused on specific applications and enabling technologies of direct relevance to NNSA mission needs. In order to convey this interest to potential respondents, some guidelines are provided herein. First, applications of interest must be such that:

1. The unclassified application domain is of interest to NNSA national security missions (see below for examples).
2. They require the integration of multiple models from different scientific and engineering disciplines some of which must be of interest to NNSA (see below for examples).
3. They ultimately involve complex computational simulations spanning significant orders of magnitude in temporal and spatial scales.

4. The associated simulations require terascale and larger computers for execution and are scalable to the thousands of processors of such systems.
5. The simulation models are integrated within algorithmic and software frameworks, the latter involving best practice software engineering methodologies.
6. The resulting simulation models lend themselves to practical verification and validation methodologies and strategies that should include the integrated use of experimental and/or observational data as a key part of model validation, as well as demonstration of numerical convergence and accuracy.
7. The simulations should facilitate making predictions of new properties and/or system dynamics that in turn can be validated by existing or planned experimental and/or observational data.

The reader familiar with the current NNSA Academic Strategic Alliance Program (ASAP) will note similarities and two key differences with PSAAP. The similarities are a focus on large-scale, 3D, multi-scale and multi-discipline integrated applications. The key differences are that: (1) the applications and associated sub-disciplines require a stronger direct connection to NNSA interests and (2) verification, validation and prediction methodologies and results must be much more strongly emphasized as research topics and demonstrated via the proposed simulations.

The following list of application areas, though not exhaustive, provides some indication of areas of interest to NNSA:

- High energy density physics/Astrophysics in the high energy density regime
- Condensed matter physics and materials science of strongly driven systems
- Design and response of engineered systems to extreme Environments, such as fire, shock and radiation
- Hydrodynamics and fluid dynamics of multiple media involving mixing, turbulence and/or reaction
- Micro/Nano scale material science and technology including synthesis, processing, integration, performance and reliability
- Chemical processes in organic materials, including energetic materials, polymers, and foams
- Materials compatibility and aging

The application areas of interest will involve and motivate research in a number of enabling sciences and technologies of interest to NNSA; examples are given below. White papers on topics marked with an "*" have been prepared by NNSA researchers and are available at this website to potential responders to the RFP to give a flavor of some of the areas of interest to the NNSA Laboratories. Successful proposals must address the first two, and many of the others.

1. Predictability in science & engineering
2. Verification & validation strategies for large scale simulations*
3. Equations of state and constitutive properties*
4. Algorithms

5. Fluid dynamics, particularly turbulence and hydrodynamics*
6. Problem solving environments (the model integration frameworks and related software tools and methodologies)
7. Computer science*
8. Computational materials science and chemistry
9. Chemical transformations including HE*
10. Material damage and failure*
11. Material stability*
12. Novel materials*
13. Nuclear properties*
14. Engineering mechanics and design (including design margins under uncertainty)
15. Particle transport*
16. Radiation effects*
17. Computational aspects of dense plasmas
18. Plasma physics*
19. Molecular dynamics
20. Design of experiments for validation, including surrogate materials and environments
21. Statistical sciences, including data integration and model calibration

There are also complex, multidisciplinary applications, while certainly appropriate areas for the application of large scale, predictive simulation, that are not of interest to NNSA for this program:

1. Response to natural and man-made threats
2. Weather
3. Climate
4. Science of natural disasters (earthquakes, tsunami, etc)
5. Infectious diseases
6. Protein dynamics
7. Eco-systems
8. Crowd behavior
9. Nuclear reactor design
10. Bioscience and Bioengineering
11. Economics and business systems
12. Logistics and agency resource deployment
13. Inertial confinement fusion (ICF) applications, ICF energy systems, and codes for design and modeling ICF phenomena and systems
14. Internal combustion engines

Additional information on the programs and interests of NNSA can be found at the following websites:

http://www.sandia.gov/NNSA/ASC/
http://www.nnsa.doe.gov/ssaa/Program_overview.htm

http://www.sandia.gov/ASC/
http://www.lanl.gov/asci/
http://www.llnl.gov/asci/
http://www.nnsa.doe.gov/

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